8.21 The Physics of Energy
Fall 2009

8.21 Lecture 14

Quantum Mechanics II
Tunneling et cetera

October 9, 2009

Quantum II

More about quantum mechanics in coordinate space

Principal aim: **Tunneling** --- To explore how particles can move through regions where classical mechanics would forbid them to be!

- Why a whole lecture devoted to this?
- Fusion in the sun: tunneling allows the sun to burn at temperatures far below the energy scale of fusion.
- Nuclear fusion on earth?
- Nuclear alpha-decay --- source of geothermal energy, and key ingredient in nuclear waste.
- Spontaneous nuclear fission.

Outline

- Reintroducing the Schrödinger equation
- Simple solutions to the Schrödinger equation
  - A square well — living classically
  - Harmonic oscillator — living in the forbidden zone
- Barrier Penetration "Lite"
- The Semi-Classical Approximation
  - What is it? Why do we use it and when can we use it?
  - Derivation
  - An application
  - Exploring the forbidden region
- Tunneling
  - The barrier penetration factor
  - The tunneling lifetime
  - Tunneling through a hump, and other applications

Review of QM notes!

- States
- Superposition
- Schrödinger equation

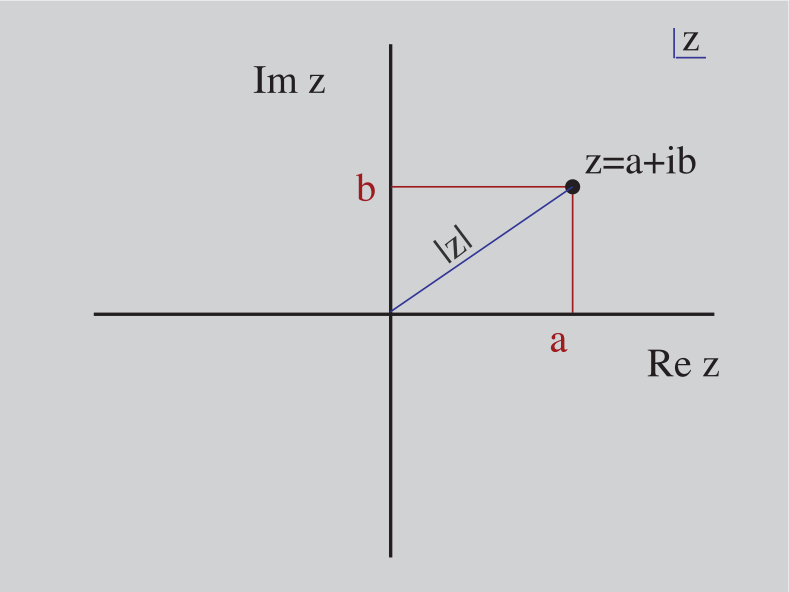
Interlude: Complex numbers

Complex number z ($z \in \mathbb{C}$) denoted

$$z = a + ib$$

where a, b are real ($a, b \in \mathbb{R}$). And, of course,

$$i^2 = -1$$



The complex plane

Multiplication of complex numbers:

$$(a + ib)(c + id) = (ac - bd) + i(ad + bc)$$

Complex conjugate

$$z^* = a - ib$$

Modulus (= length) of a complex number

$$|z| = \sqrt{z^* z} = \sqrt{a^2 + b^2}$$

Modulus and phase representation

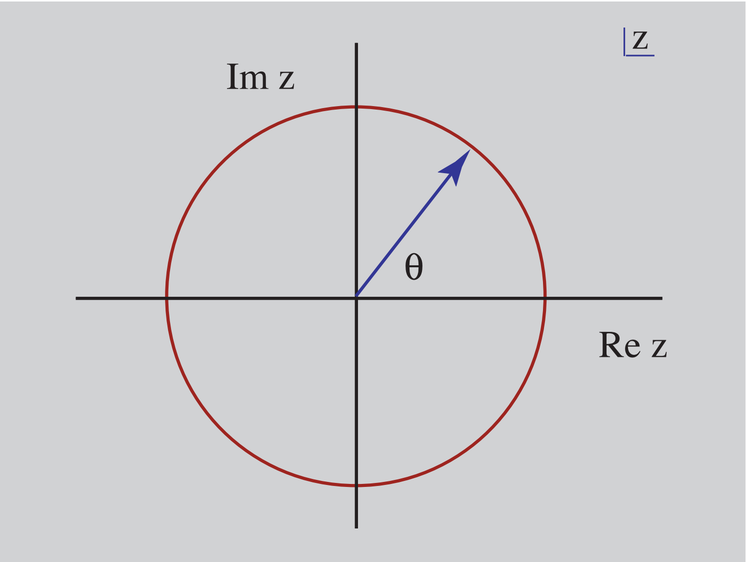
$$\begin{aligned} z = a + ib &= |z| \left(\frac{a}{\sqrt{a^2+b^2}} + i \frac{b}{\sqrt{a^2+b^2}} \right) \\ &= |z| \left(\cos\theta + i \sin\theta \right) \\ &= |z| \, e^{i\theta} \end{aligned}$$

where $\tan\theta = b/a$.

"Modulus" — $|z|$ "Phase" — θ

Sometimes people refer to $e^{i\theta}$ as a "pure phase".

And it can be envisioned as a unit vector making an angle θ with the real axis in the complex plane.

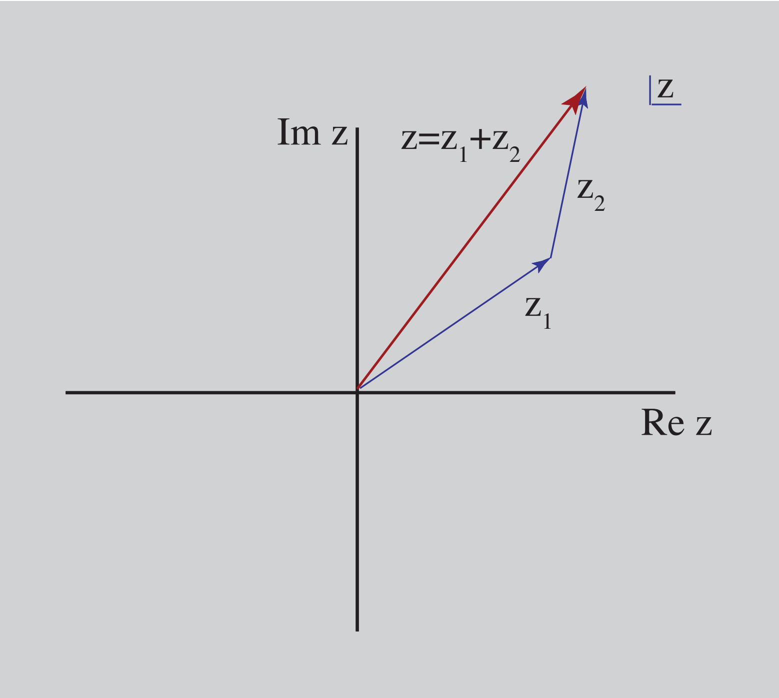


Note the famous identities:

$$\begin{aligned} \cos\theta &= \frac{1}{2} \left(e^{i\theta} + e^{-i\theta} \right) \\ \sin\theta &= \frac{1}{2i} \left(e^{i\theta} - e^{-i\theta} \right) \end{aligned}$$

Adding complex numbers is both algebraically and geometrically identical to adding vectors in the plane.

$$\begin{aligned} z_1 &= a_1 + i b_1 \\ z_2 &= a_2 + i b_2 \quad \text{so} \\ z = z_1 + z_2 &= (a_1 + a_2) + i(b_1 + b_2) \end{aligned}$$



Logical sequence leading to Schrödinger equation

(1) De Broglie waves: $\Psi(x,t) = e^{(ipx - iEt)/\hbar}$

Wavelength $\lambda = \dfrac{h}{p}$ Frequency $\nu = \dfrac{E}{h}$

ELECTRON DIFFRACTION

RADIATION IN ATOMIC TRANSITIONS

(2) Association of energy and momentum with derivatives

$$-i\hbar\frac{\partial}{\partial x}\left(e^{(ipx-iEt)/\hbar}\right) = p\left(e^{(ipx-iEt)/\hbar}\right)$$

$$i\hbar\frac{\partial}{\partial t}\left(e^{(ipx-iEt)/\hbar}\right) = E\left(e^{(ipx-iEt)/\hbar}\right)$$

(3) Energy and momentum:

$$E = \frac{p^2}{2m}$$

$$\Downarrow$$

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$$

(4) Add a potential

$$E = \frac{p^2}{2m} + V(x) \iff i\hbar\frac{\partial\Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi$$

(5) Definite energy: $\Psi(x,t) \Rightarrow e^{-iEt/\hbar}\,\psi(x)$

$$\boxed{E\,\psi(x) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x)}$$

An aside on time dependent processes in QM

- QM $\Rightarrow$ probabilities
- Per unit time:

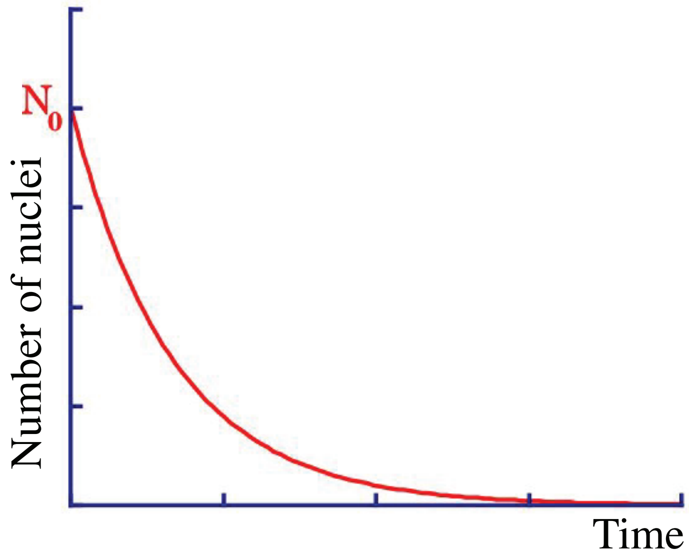
$$\frac{dP}{dt} \equiv \frac{1}{\tau}$$

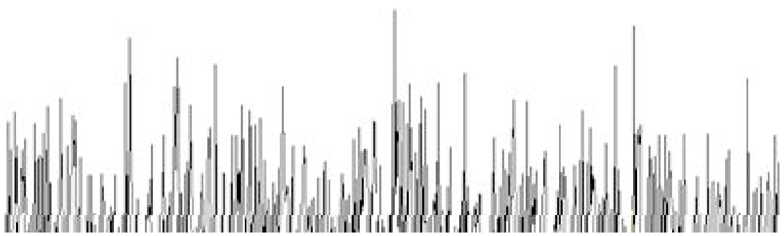
- Process like radioactive decay:

$$\frac{dN}{dt} = -\frac{dP}{dt}N = -\frac{1}{\tau}N$$

- $$N(t) = N_0 e^{-t/\tau}$$

- $\tau \equiv$ **lifetime**



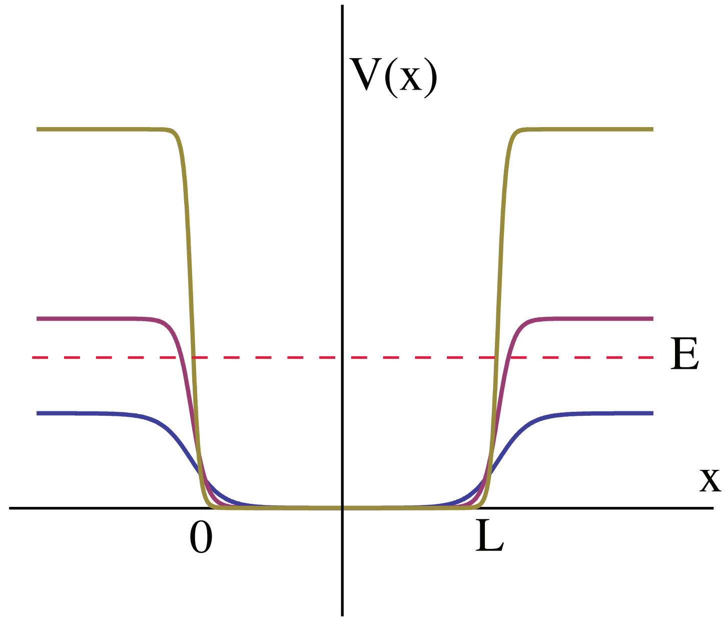


Events are random, with no correlations except for $\langle \Delta t \rangle = \tau$

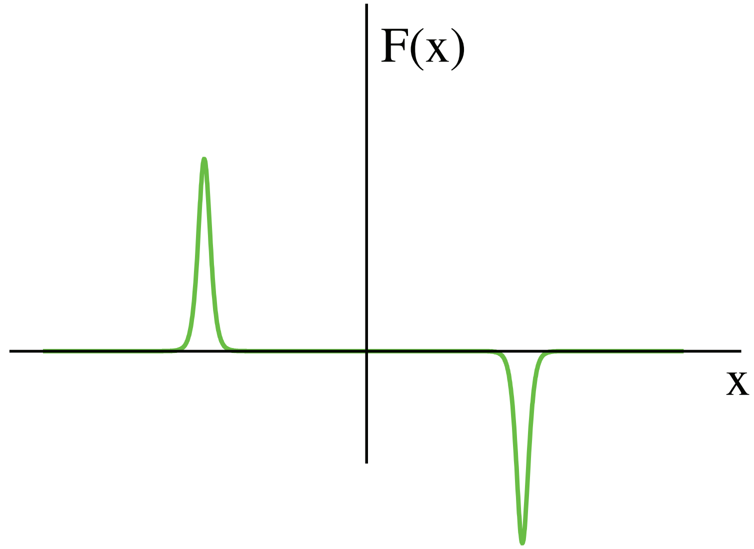
Simple solutions to Schrödinger's equation and their (wierd) interpretation

Example 1: Life inside a potential well: "the square well"

- How to make one. Build a wall and let its height go to infinity.
- Sharp strong force.
- Keeps the particle between the walls.
- Particle lives only in the classically allowed region.



- $\psi(0) = \psi(L) = 0$
- $-\frac{\hbar^2}{2m}\psi''(x) = E\psi(x)$
- $\psi(x) = \sqrt{2}L \sin(n\pi x/L), \quad n = 1, 2, \ldots$
- $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$



Solving the square well — carefully —

- $V(x) = 0$ inside $\Rightarrow$ two solutions to Schrödinger equation,

$$\psi_\pm(x) \propto e^{\pm ipx/\hbar}$$

with $p = \sqrt{2mE}$.

- But $\psi(0) = 0$. Neither solution satisfies this, but the superposition, $\psi_+ - \psi_-$, does.
- So

$$\psi(x) \propto \left(e^{ipx/\hbar} - e^{-ipx/\hbar}\right) = N \sin px/\hbar$$

where N is a "normalization constant" to be determined.

- What about $\psi(L) = 0$? Since $\sin n\pi = 0$, we conclude

$$pL = p_n L = n\pi\hbar \quad \text{and therefore, } E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

Finally, the Schrödinger dwavefunction must be normalized so $\int_0^L dx|\psi_n(x)|^2 = 1$, so that probability to find the particle somewhere is unity,

$$N^2 \int_0^L dx \sin^2 n\pi x/L = 1 \quad \Rightarrow \quad N = \sqrt{\frac{2}{L}}$$

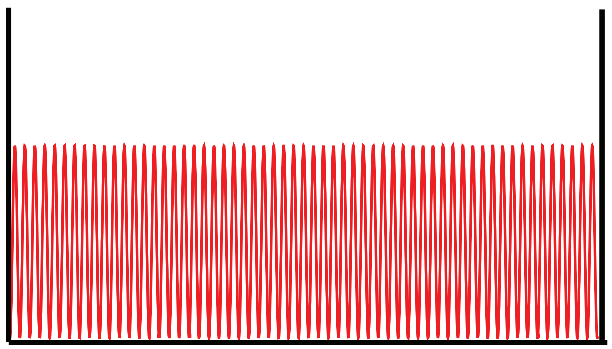
Finally

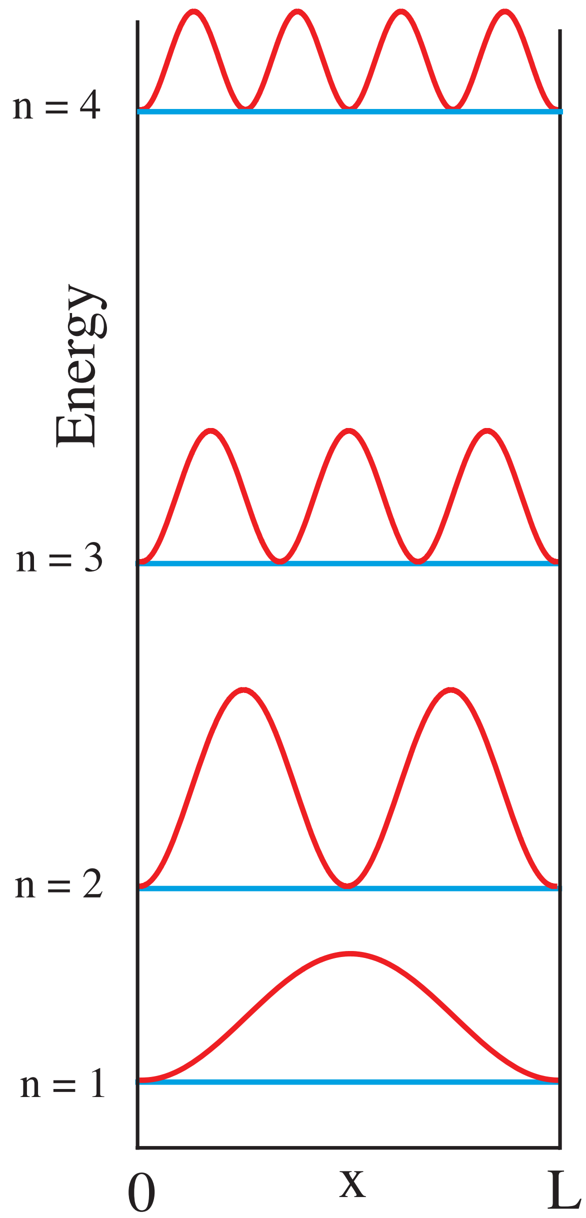
$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin n\pi x/L$$

- Energy levels $n = 1, 2, 3, 4.$
- Squared wavefunctions give probability per unit x,

$$\frac{d\,\text{Probability}}{dx} = |\psi(x)|^2$$

- Particle $\leftrightarrow$ standing wave
- Particle still lives between the walls.
- Very highly excited state — equally probable everywhere inside, but zero outside.

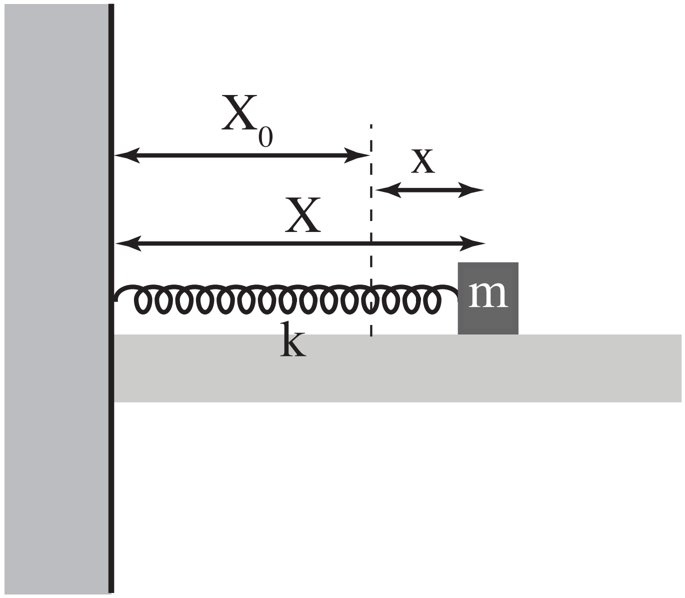




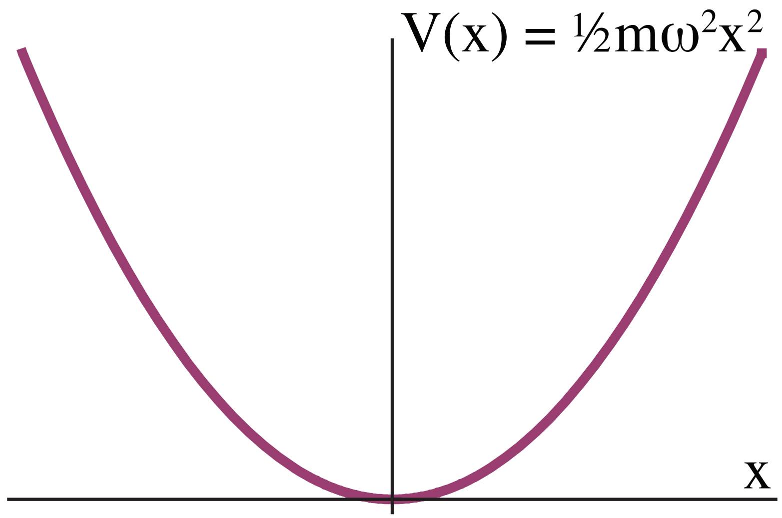
Example: Life in the forbidden zone — the harmonic oscillator

Quantum particle on a spring:

- x is distance from equilibium



- $F = -kx = -m\omega^2 x, \quad \omega = \sqrt{k/m}$
- $V(x) = \frac{1}{2} m\,\omega^2 x^2$



Results from Unit 6

- $E_n = (n + 1/2)\hbar\omega, \; n = 0, 1, 2, \ldots.$

Now let's look closer at the wavefunctions...

Quantum harmonic oscillator

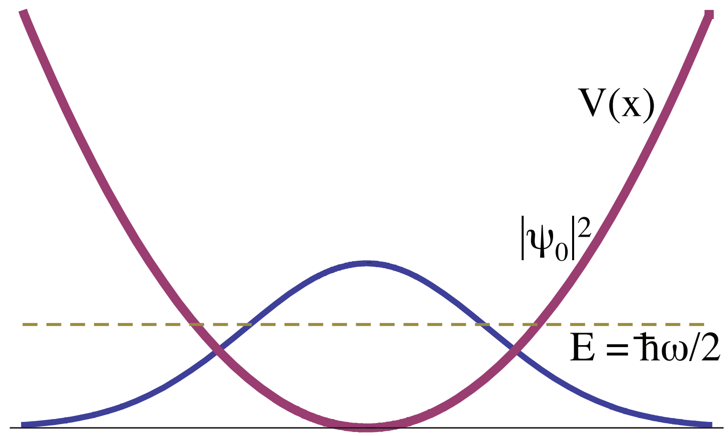
- Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_E(x)+\frac{1}{2}m\omega^2x^2\psi_E(x)=E\psi_E(x)$$

- Differential equation — not our job — though it isn't hard.
- Solutions are polynomials in x multiplying "Gaussians", $e^{-\frac{1}{2}\alpha x^2}$. Try the simplest one:

$$\psi_{\text{trial}}(x)=N\exp\left(-\frac{1}{2}\alpha x^2\right)$$

$$\psi_0(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}e^{\left(-\frac{m\omega x^2}{2\hbar}\right)}$$



Showing that ψ_{trial} is a solution:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\exp\left(-\frac{1}{2}\alpha x^2\right)+\frac{1}{2}m\omega^2x^2\exp\left(-\frac{1}{2}\alpha x^2\right) = E\exp\left(-\frac{1}{2}\alpha x^2\right)$$

$$-\frac{\hbar^2}{2m}(\alpha^2x^2-\alpha)+\frac{1}{2}m\omega^2x^2 = E$$

$$\alpha = m\omega/\hbar$$

$$E = \frac{\alpha\hbar^2}{2m}=\frac{1}{2}\hbar\omega$$

Normalizing it:

$$\int_{-\infty}^{\infty} dx\,|\psi(x)|^2 = 1$$

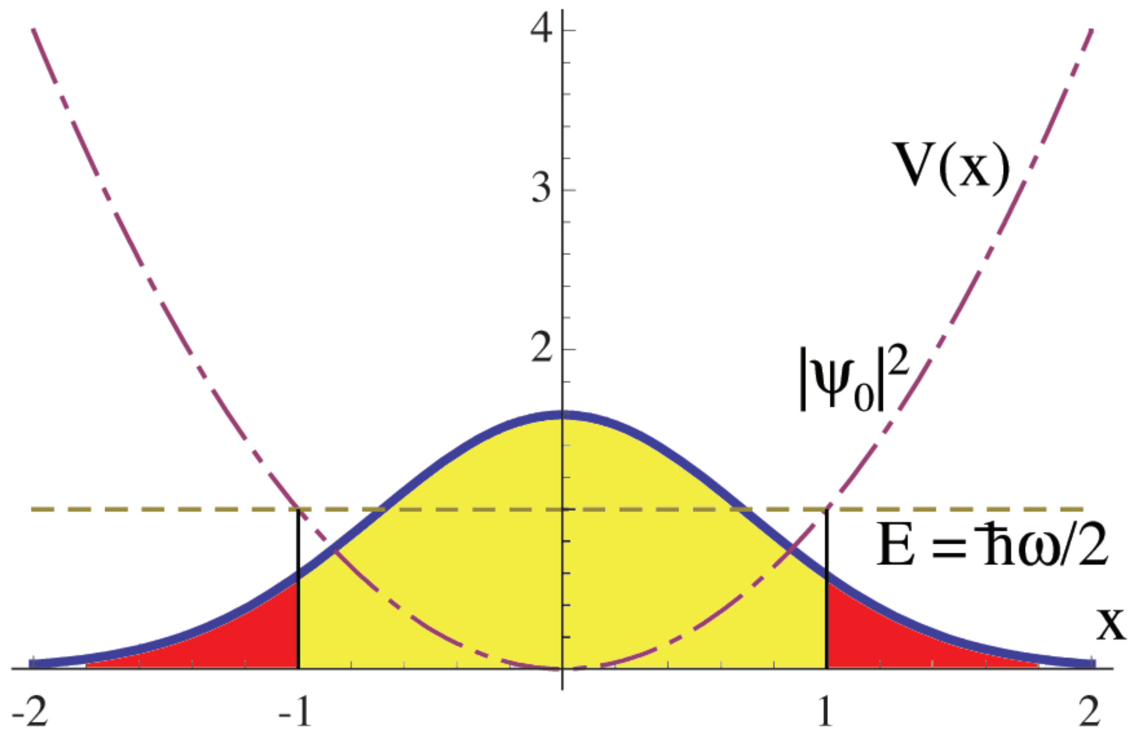
$$N^2\int_{-\infty}^{\infty} dx e^{-\alpha x^2} = 1$$

$$N = \sqrt[4]{\frac{m\omega}{\pi\hbar}}$$

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{\left(-\frac{m\omega x^2}{2\hbar}\right)}$$

Plot it!

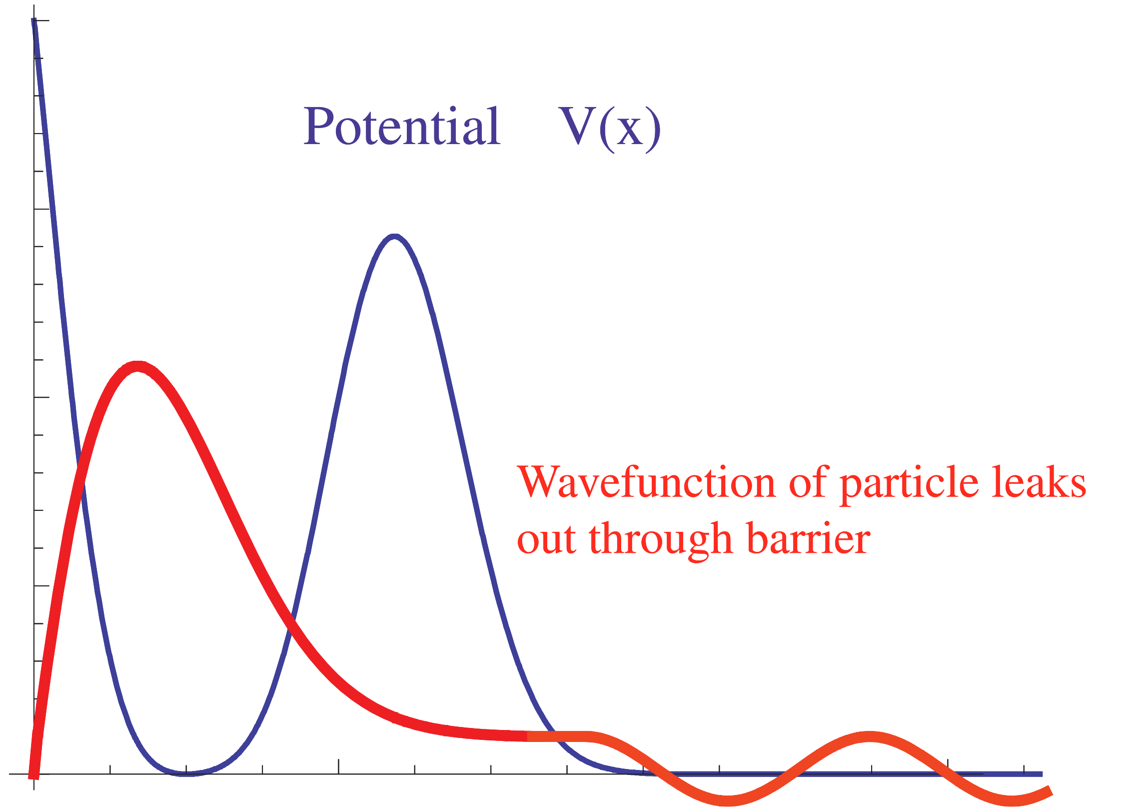
- Solid line is profile of $|\psi_0(x)|^2$
- Dashed-dot line is potential.
- It equals the total energy at $x = \sqrt{\hbar/m\omega}$
- Yellow measures probability in classically allowed region
- Red measures probability in classically forbidden region



x in units of $\sqrt{\hbar/m\omega}$

- Significant probability to be found in forbidden zone.
- What are we to make of this?

- If the wavefunction changes smoothly as it enters a forbidden zone, then it will also change smoothly as it exits.
- So the particle has a probability to tunnel through a forbidden zone, out of a classical trap.
- Prediction of quantum mechanics — must be verified by experiment! And is!



Need a way to compute the probability of tunneling out of a trap (or into a potential well through a wall).

Leads us to the semiclassical approximation

Barrier Penetration "Lite"

- Take idea seriously and look at constant potentials
- STEP 1: $V(x) = 0$

  $\psi_{\pm p}(x) = e^{\pm ipx/\hbar}$ A plane wave moving right (+) or left (−)

  $p = \sqrt{2mE}$

  Satisfies free Schrödinger equation... $-\frac{\hbar^2}{2m}\psi''_{\pm p}(x) = E\psi_{\pm p}(x)$

- STEP 2: $V(x) = V_0$, with $E > V_0$.

  $\psi_{\pm p}(x) = e^{\pm ipx/\hbar}$

  $p = \sqrt{2m(E - V_0)}$

  Satisfies interacting Sch. eq.... $-\frac{\hbar^2}{2m}\psi''_{\pm p}(x) + V_0\psi_{\pm p}(x) = E\psi_{\pm p}(x)$

- STEP 3: $V(x) = V_0$, with $E < V_0$.

The "momentum" becomes imaginary:

$$\begin{aligned} \frac{p^2}{2m} &= E - V_0 < 0 \\ p(x) \equiv i\kappa(x) &= i\sqrt{2m(V_0 - E)} \end{aligned}$$

And the wavefunctions become exponentials:

$$\psi_{\pm\kappa}(x) = e^{\pm\kappa x/\hbar} = e^{\pm\frac{1}{\hbar}\sqrt{2m(V_0-E)}x}$$

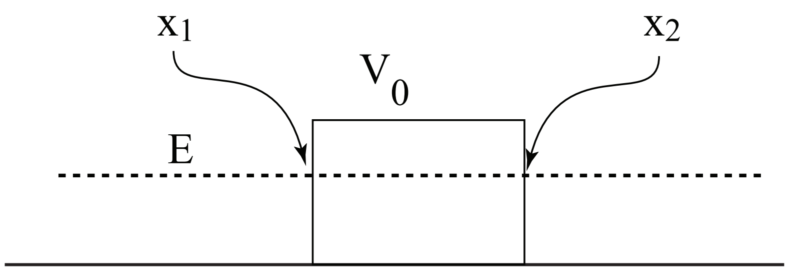
Which satisfies interacting Sch. eq...

$$\begin{aligned} Ee^{\pm\kappa x/\hbar} &= \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right)e^{\pm\kappa x/\hbar} \\ &= \left(-\frac{\kappa^2}{2m} + V_0\right)e^{\pm\kappa x/\hbar} \end{aligned}$$

$$\psi_{\pm\kappa}(x) = e^{\pm\kappa x/\hbar} = e^{\pm\frac{1}{\hbar}\sqrt{2m(V_0-E)}x}$$

Amplitude to pass through barrier

$$A(E) = e^{-\frac{1}{\hbar}\sqrt{2m(V_0-E)}(x_2-x_1)}$$

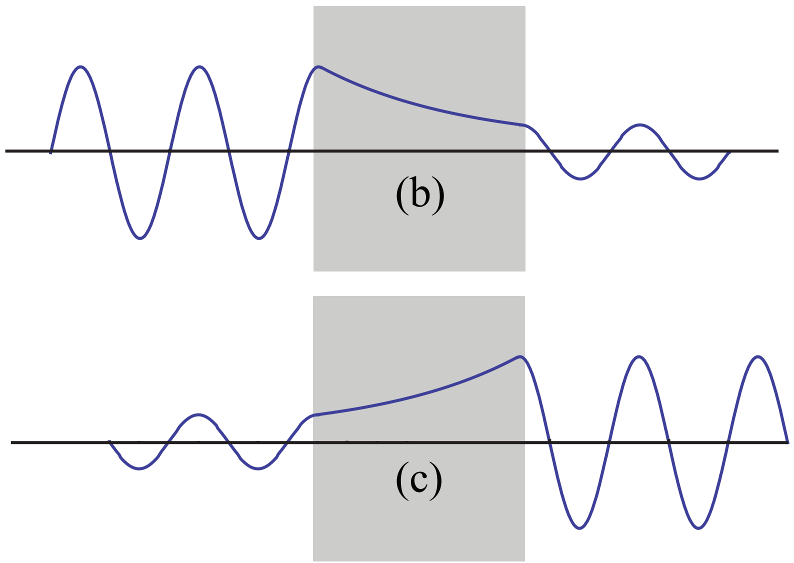


(a)

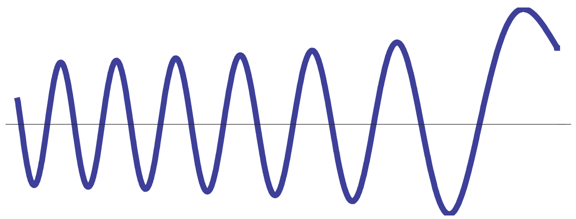
Probability to pass through barrier

$$P(E) = |A(E)|^2 = e^{-\frac{2}{\hbar}\sqrt{2m(V_0-E)}(x_2-x_1)}$$

"Barrier penetration factor"


(b)
(c)

What happens when $V(x)$ is not constant?

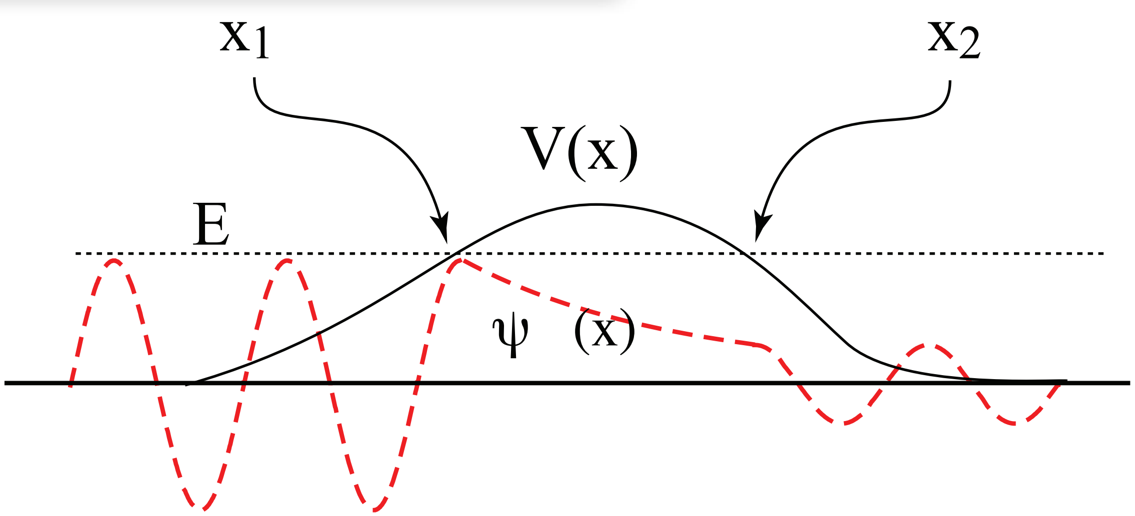


- Slowly varying deBroglie wavelength in allowed regions

  $$\text{deBroglie wavelength} = \frac{\hbar}{p} \longrightarrow \frac{\hbar}{p(x)} = \frac{\hbar}{\sqrt{2m(E-V(x))}}$$

- $\kappa \longrightarrow \kappa(x) = \sqrt{2m(V(x)-E)}$

$$P(E) = \exp\left(-\frac{2}{\hbar}\int_{x_1}^{x_2} dx\sqrt{2m(V(x)-E)}\right)$$



Outline

- Reintroducing the Schrödinger equation
- Simple solutions to the Schrödinger equation
  - A square well — living classically
  - Harmonic oscillator — living in the forbidden zone
- Barrier Penetration "Lite"
- The Semi-Classical Approximation
  - What is it? Why do we use it and when can we use it?
  - Derivation
  - An application
  - Exploring the forbidden region
- Tunneling
  - The barrier penetration factor
  - The tunneling lifetime
  - Tunneling through a hump, and other applications

Semiclassical Approximation

General solution?

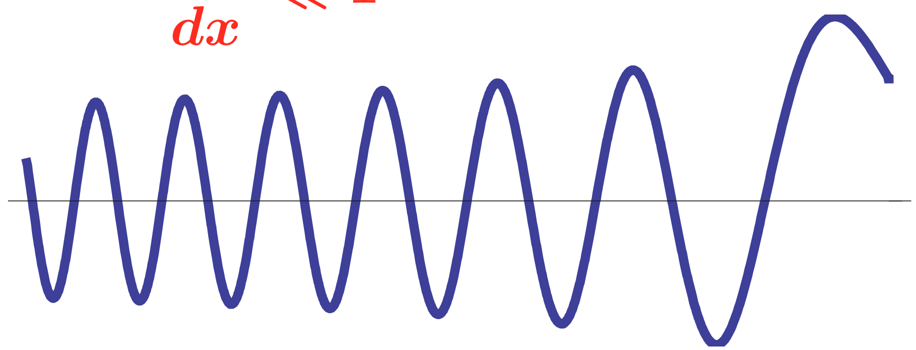
- Too hard!
- Can solve Schrödinger equation for V = constant
- Attempt a modified de Broglie wave for a smoothly varying potential.

Constant potential: $p = \sqrt{2m(E - V_0)}$ $\quad \lambda\!\!\!^{-} = \hbar/p$

Spatially varying potential: $V_0 \to V(x)$ $\quad \boxed{\lambda\!\!\!^{-} = \hbar/\sqrt{2m(E - V(x))}}$

Maybe this will work if $\lambda\!\!\!^{-}(x)$ changes slowly with x,

$$\frac{d\lambda\!\!\!^{-}}{dx} \ll 1$$



Semiclassical?

Turns out $d\lambda\!\!\!^{-}/dx \ll 1$ is the same as $\hbar$ small $\longrightarrow$ "Semiclassical"

$$\psi_{\text{trial}} \equiv \exp\left(\frac{i}{\hbar}\sigma(x)\right)$$

Substitute into equation:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(e^{i\sigma/\hbar}\right) + V(x)\left(e^{i\sigma/\hbar}\right) = E\left(e^{i\sigma/\hbar}\right)$$

$$\frac{1}{2m}\sigma'^2(x) - \frac{i\hbar}{2m}\sigma''(x) + V(x) = E$$

$$\boxed{\sigma'(x) = \pm\sqrt{2m(E - V(x))} \equiv \pm p(x)}$$

$$\sigma(x) = \pm\int^x dy\; p(y) + \text{ constant} \qquad \psi_\pm \propto \exp\left(\pm\frac{i}{\hbar}\int^x dy\;\sqrt{2m(E - V(y))}\right)$$

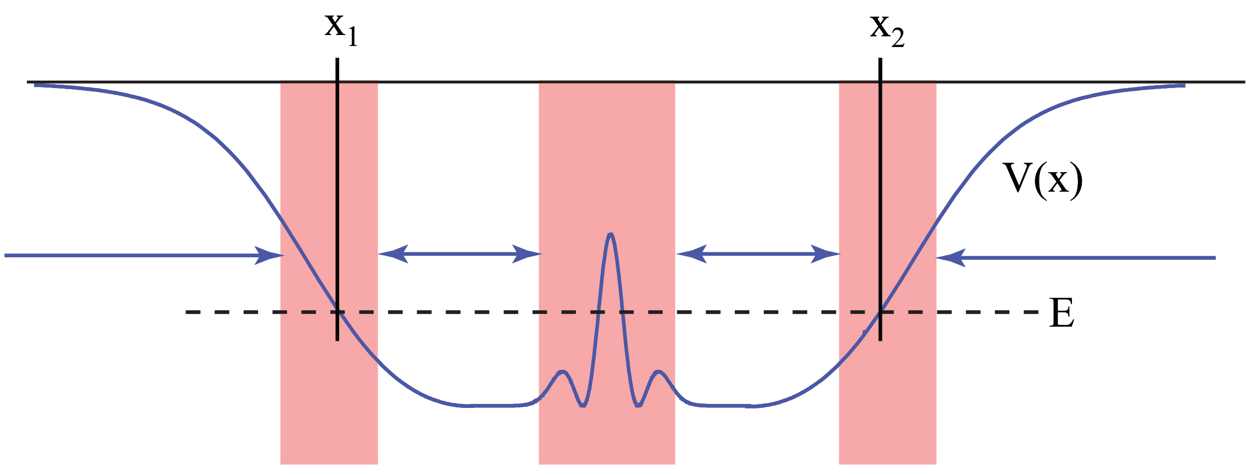
Before applying: Interpret? What have we ignored?

$$|i\hbar\sigma''| \ll |\sigma'|^2$$

$$\left|\frac{\hbar\sigma''}{\sigma'^2}\right| = \frac{d}{dx}\left|\frac{\hbar}{\sigma'(x)}\right| = \frac{d}{dx}\left|\frac{\hbar}{p(x)}\right| = \frac{d}{dx}|\lambda\!\!\!^{-}| \ll 1$$

So the "semiclassical approximation" works when the de Broglie wavelength is slowly changing. Where does it break down?

- Classical turning points, where $p(x) = 0$.
- Potentials where $V(x)$ changes too rapidly



Example: Add $V(x)$ to a box...

- First steps are just like $V = 0$ case: take superposition of $\psi_{\pm}(x)$ to vanish at $x = 0$,

$$\psi(x) = N \sin \frac{1}{\hbar} \int_{0}^{x} dy \sqrt{2m(E - V(y))}$$

- But need $\psi(L) = 0$, so

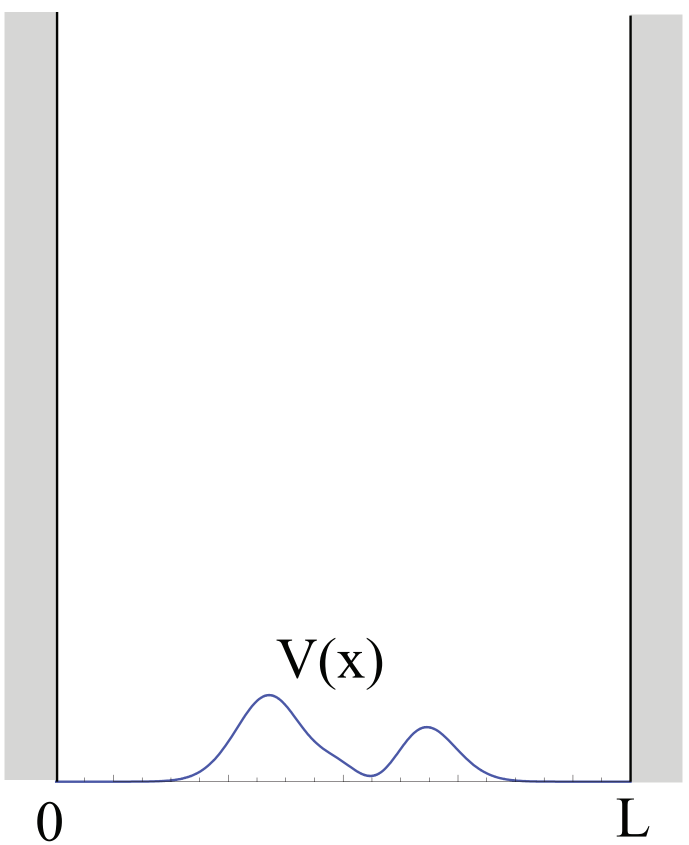
$$\int_{0}^{L} dy \sqrt{2m(E - V(y))} = n\pi\hbar$$

- Or more beautifully (and briefly)

$$\int_{\text{period}} p\, dx = nh$$

because the integral over $[0, L]$ covers 1/2 of the classical period.

Bohr-Sommerfeld Quantization Condition



What about classically forbidden region?

- There was nothing in our "derivation" that depended on $E > V(x)$, so let's try $V(x) > E$!

$$p(x) = \sqrt{2m(E - V(x))} = i\sqrt{2m(V(x) - E)} \equiv i\kappa(x), \text{ and}$$
$$\psi_\pm(x) = \exp\left(\pm\frac{1}{\hbar}\int^x dy\kappa(y)\right) = \exp\left(\pm\frac{1}{\hbar}\int^x dy\sqrt{2m(V(y) - E)}\right)$$

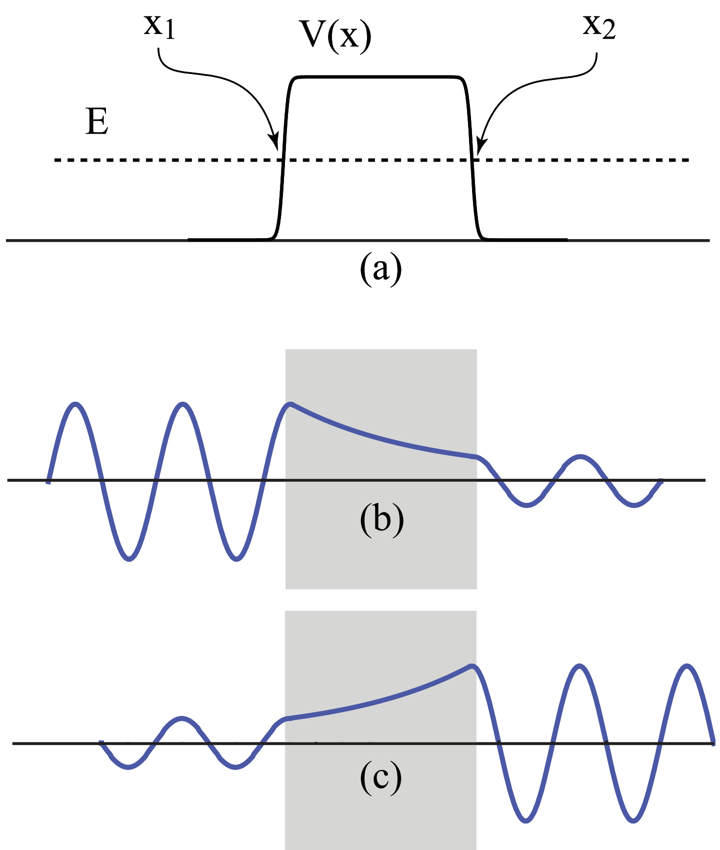
- So wavefunctions either decrease or blow up exponentially in classically forbidden regions!

A particle confronts a barrier (a) without enough energy to get over it.

- Probability to penetrate decreases exponentially with distance, (b).
- What about increasing? Look at (c).

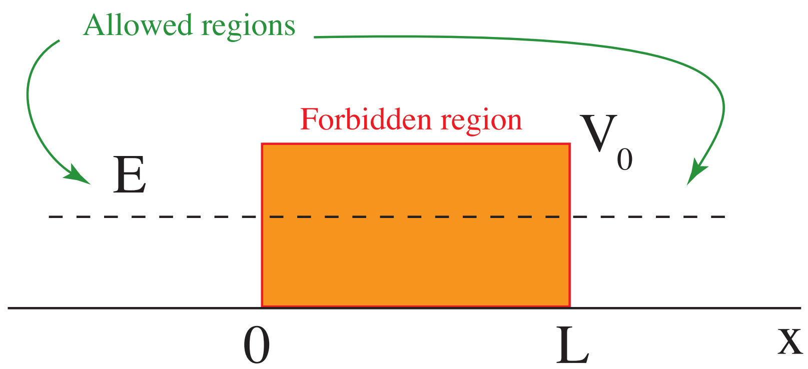
Barrier penetration factor

$$P(E) = \exp(-\frac{2}{\hbar}\int_{x_1}^{x_2} dy\sqrt{2m(V(x) - E)})$$



Simplest example: A "Square barrier" $V(x) = \begin{cases} 0 & \text{for } x < 0,\ x > L; \\ V_0 & \text{for } 0 \leq x \leq L \end{cases}$

$$P(E) = \exp(-\frac{2}{\hbar}\sqrt{2m(V_0 - E)}L)$$



- 1 eV electron incident on a 2 eV barrier 1 Å wide

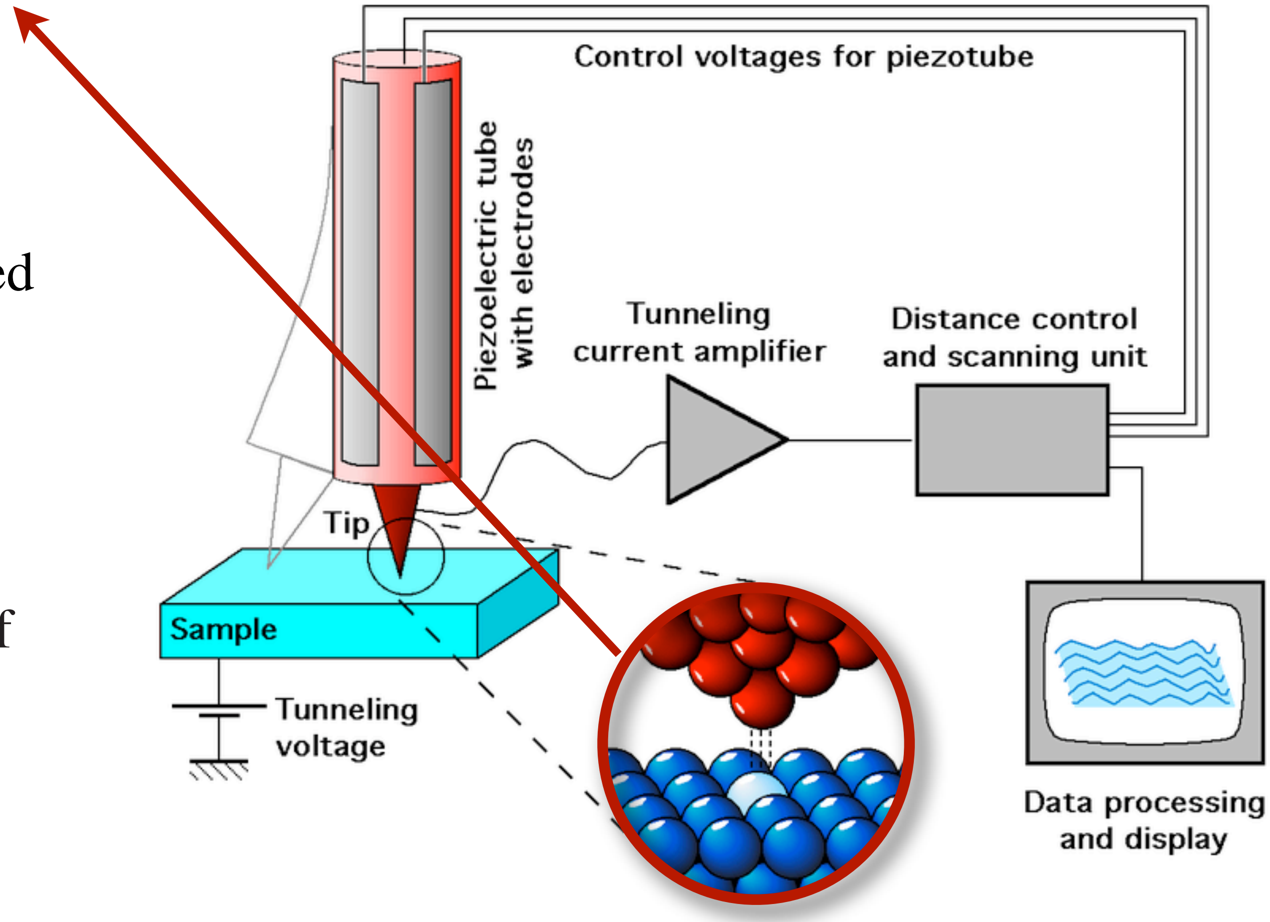
$$\begin{aligned} P &= \exp\left(-\frac{2}{1.05 \times 10^{-34}} \times 10^{-10} \times \sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19}}\right) \\ &\approx e^{-1} = 0.37 \end{aligned}$$

- Proton under the same conditions? $m_p \sim 2000 \times m_e$ so a proton has a probability $P \approx \exp(-\sqrt{2000}) \approx 4 \times 10^{-20}$ to tunnel!

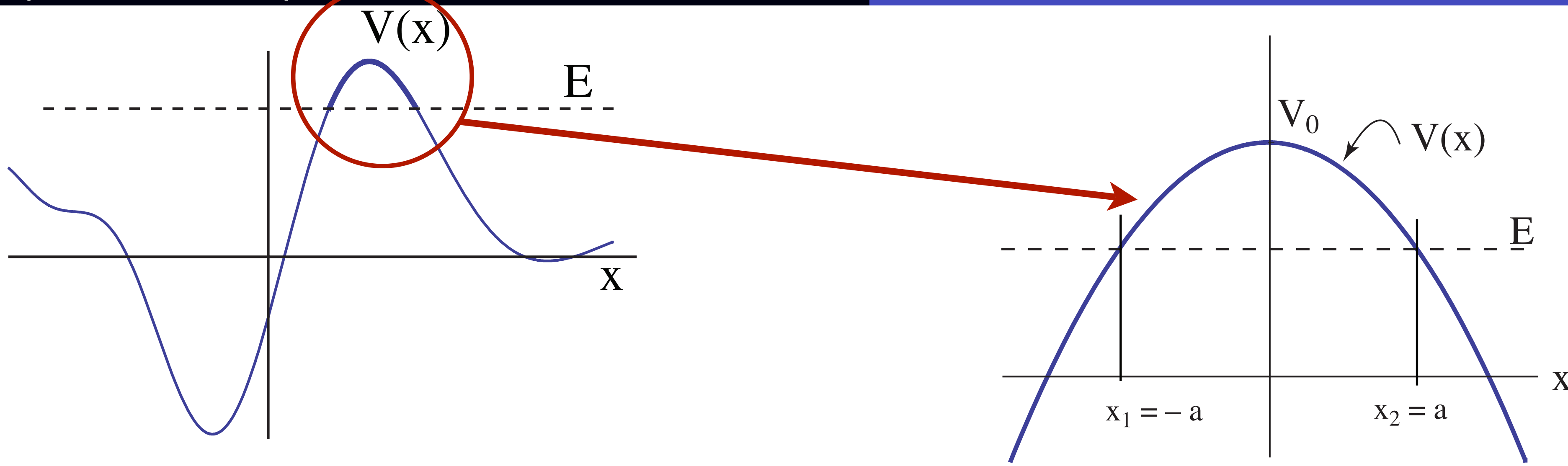
  Practical consequences: When two pieces of metal are brought very close to one another, electrons can tunnel from one to the other (this is the physical basis of the *scanning tunneling microscope* or STM), but the atoms themselves which are even heavier than protons stay put.

How an S(canning) T(unneling) M(icroscope) works...

- Red is tip of probe
- Blue is surface being probed
- Gap between is forbidden zone for electrons
- Tunneling rate depends exponentially on the size of gap.
- Allows very precise tomography of surface



Courtesy of Science of Spectroscopy.



Close to the top of a (any) smooth barrier:

- Near the top: $V(x) = V_0 - \frac{1}{2}kx^2 = V_0 - \frac{1}{2}m\omega^2 x^2$
- Classical turning points (boundaries of forbidden zone)

$$E = V(\pm a) \Rightarrow a = \sqrt{\frac{2}{k}(V_0 - E)}$$

$$\begin{aligned} P(E) &= \exp\left(-\frac{2}{\hbar}\int_{-a}^{a} dx \sqrt{2m\left(V_0 - \frac{k}{2}x^2 - E\right)}\right) \\ &= \exp\left(-\frac{\pi(V_0 - E)}{\hbar\omega}\right) \end{aligned}$$

Height of barrier

Width of barrier $\propto 1/\hbar\omega$

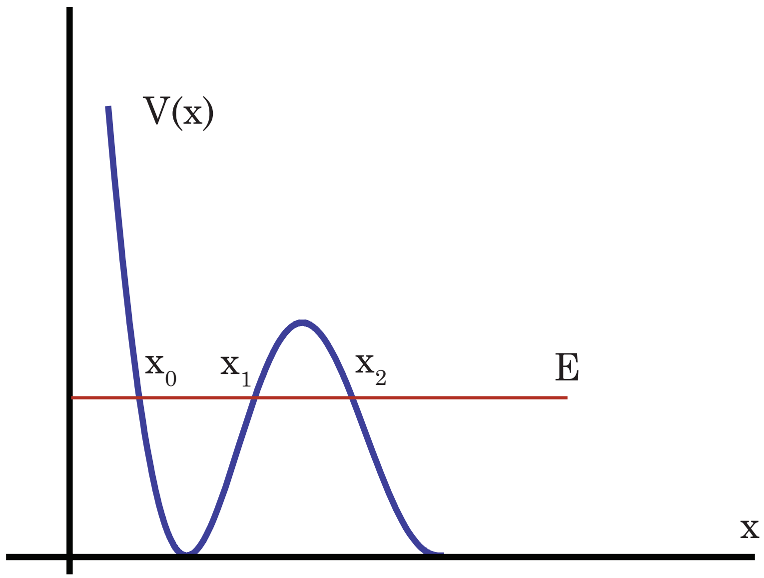
Tunneling lifetimes:

- Barrier factor, $P(E)$, measures probability of tunneling per encounter.
- To get lifetime for tunneling, we need the number of encounters per second.
- Estimate: once every period of the classical motion, $T(E)$.

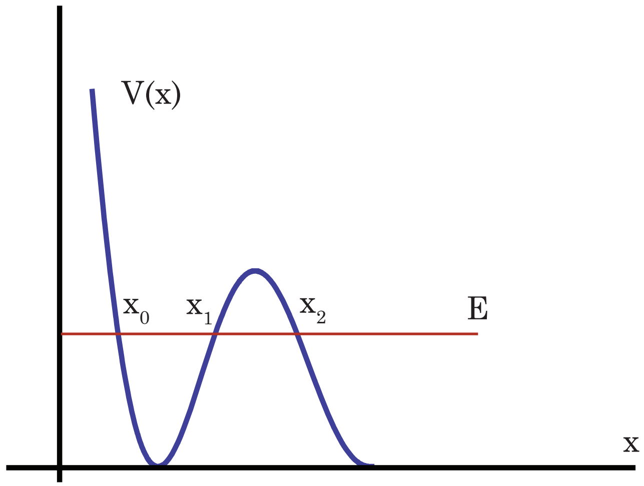
$$T(E) = \int_{\text{period}} dt = \int_{\text{period}} \frac{dx}{\dot{x}}$$

$$= 2 \times \int_{x_0}^{x_1} \frac{dx}{v(x)}$$

$$= \boxed{2\int_{x_0}^{x_1} dx \sqrt{\frac{m}{2(E - V(x))}}}$$



Putting all together



- Probability per unit time of tunneling

$$\frac{dP}{dt} = \frac{P(E)}{T(E)}$$

- Interpret: Number of atoms (or nuclei, or ...) decaying per unit time,

$$\frac{dN}{dt} = \frac{dP}{dt} \times N(t) = \frac{P(E)}{T(E)} N(t) \equiv \frac{1}{\tau} N(t)$$

Where τ is the lifetime

- Finally,

$$\boxed{\tau = \frac{T(E)}{P(E)} = 2 \int_{x_0(E)}^{x_1(E)} dx \frac{m}{\sqrt{2(E - V(x))}} \times \exp\left(\frac{2}{\hbar} \int_{x_1(E)}^{x_2(E)} dx \sqrt{2m(V(x) - E)} \right)}$$

Summary

- Wave functions don't end at the boundary of classical motion. They leak into forbidden regions

- Schrödinger equation difficult in general ⇒ semiclassical approximation

  Slowly changing deBroglie wavelength: $d\lambda\!\!\!^{-}/dx \ll 1$

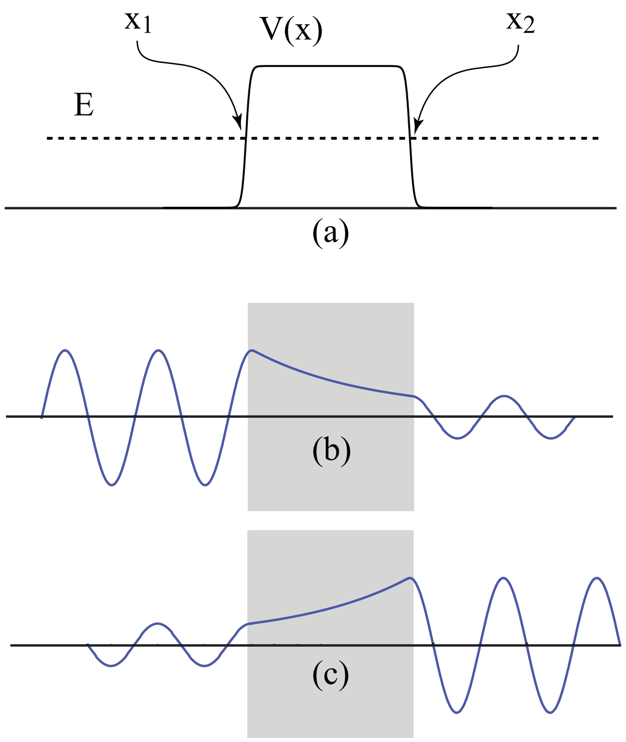
- $$\begin{aligned} \psi(x) &= c_+\psi_+(x) + c_-\psi_-(x) \\ &= c_+ \exp\left(\frac{i}{\hbar}\int^x p(y)dy\right) + c_- \exp\left(-\frac{i}{\hbar}\int^x p(y)dy\right) \end{aligned}$$

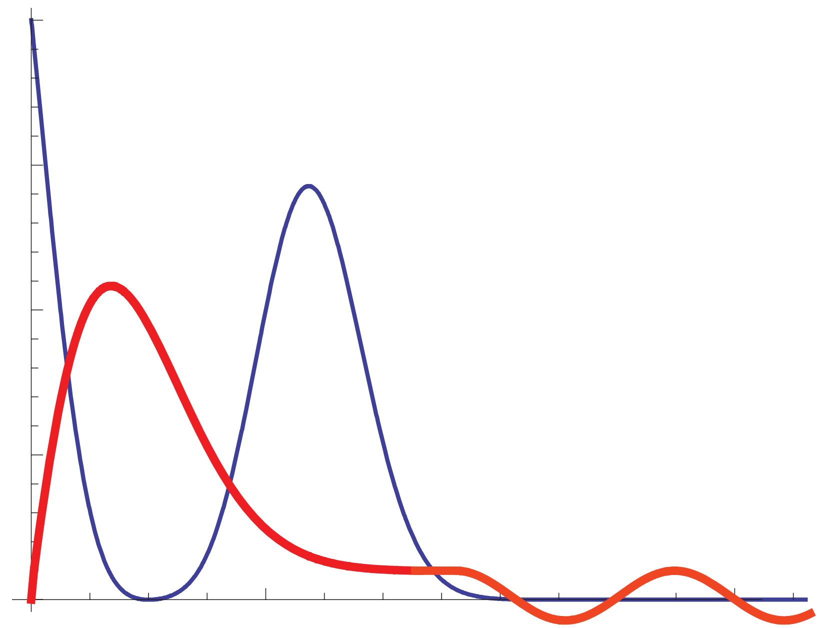
  $p = \sqrt{2m(E - V(x))}$ – classical momentum

- Classically forbidden region $p(x) \to i\kappa(x) = i\sqrt{2m(V(x)-E)}$

$$\psi_{\pm}(x) \propto \exp\left(\pm\frac{1}{\hbar}\int^{x} dy\,\kappa(y)\right)$$

- $P(E) = |\mathcal{A}(E)|^2 = \exp\left(-\frac{2}{\hbar}\int_{x_1}^{x_2} dx\sqrt{2m(V(x)-E)}\right)$,





- Period of classical motion — how often the barrier is attacked

$$T(E) = 2\int_{x_0(E)}^{x_1(E)} dx \sqrt{\frac{m}{2(E - V(x))}}$$

- Semiclassical lifetime

$$\tau = \frac{T(E)}{P(E)} = 2\int_{x_0(E)}^{x_1(E)} dx \sqrt{\frac{m}{2(E - V(x))}} \times \exp\left(\frac{2}{\hbar}\int_{x_1(E)}^{x_2(E)} dx \sqrt{2m(V(x) - E)}\right)$$